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QSARs of Some 5- or 6-Methyl-2-Substituted Benzoxazoles/Benzimidazoles against *Candida albicans*

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Abstract: QSAR analysis of some 5- or 6-methyl-2-substituted benzoxazoles/ benzimidazoles was studied for the antifungal activity against *C. albicans* using Hansch analysis. Prediction for the lead optimization in this QSAR analysis was described by the description of various hydrophobic, electronic, steric and structural parameters related to positions R_1 , R_2 , R_5 , R_6 , X, Y. The cross-validation method was also applied to the data set in order to prove the predictive power by using the BILIN statistical software. The resulting QSAR revealed that substitution at position Y with the CH_2 group was significant for the improved antifungal activity. Moreover, hydrophobic properties of the substituents at position R_2 are indicative for the antifungal activity against *C. albicans*.

Key Words: Benzoxazole, Benzimidazole, Antifungal activity, QSAR, Hansch analysis

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